Data acquisition developments and collaborations at Daresbury Laboratory

Collaboration

- Collaboration not necessarily easy
- Communication is key
- Best to practise with friends first
- Will describe couple of developments based on collaborations
  - PXGEN++
  - DNA

PX Objectives

- PXGEN out of date and hard to update.
- Robust replacement offering greater functionality.
- Uniform interface across stations, detectors, cameras etc.
- Simple GUIs that make set up and data collection easy.
- Automation wherever possible.
- Link data acquisition and processing.
- Flexibility to cope with future changes.
- Remote monitoring and control.

Daresbury Objectives

- Cross facility group collaboration.
- Possible deployment to DIAMOND.
- Plug and play construction.
- Scripting language to facilitate easy configuration of experiments.
- Distributed solution.

Strategy

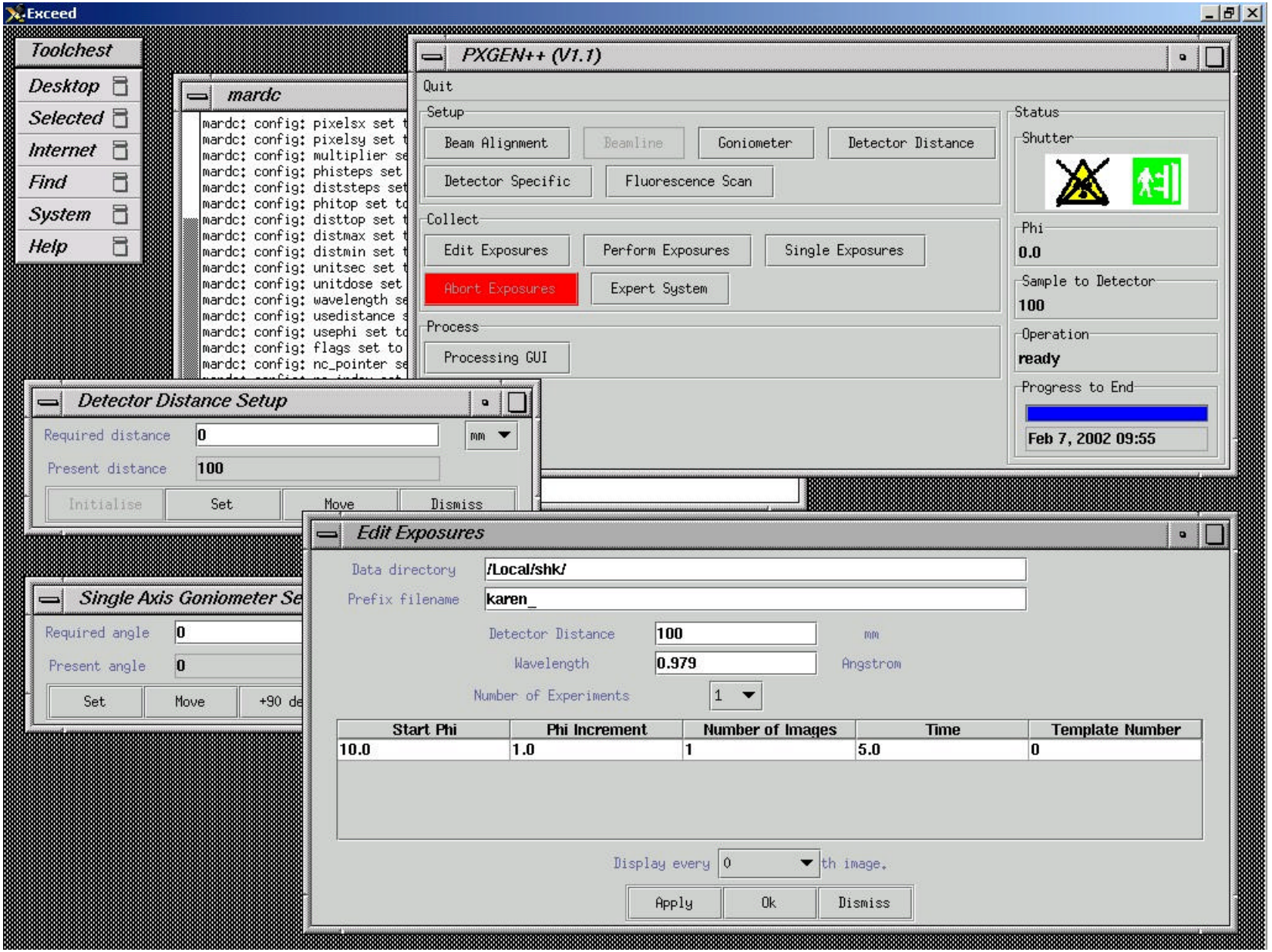
- Inter project collaboration.
  - PX, NCD, XRS, XRD, VUV-IR.
- Incremental and iterative development.
- Largely object oriented development. Java, C++ and C.
- Classes to represent real beam line hardware e.g. detectors, cameras, tables, mirrors etc.
- Use interfaces to give plug and play.
- Use CORBA to enable distribution.
- Provide common ‘look and feel’ where appropriate.
- Configuration of objects via XML files.

Advantages to in-house collaboration

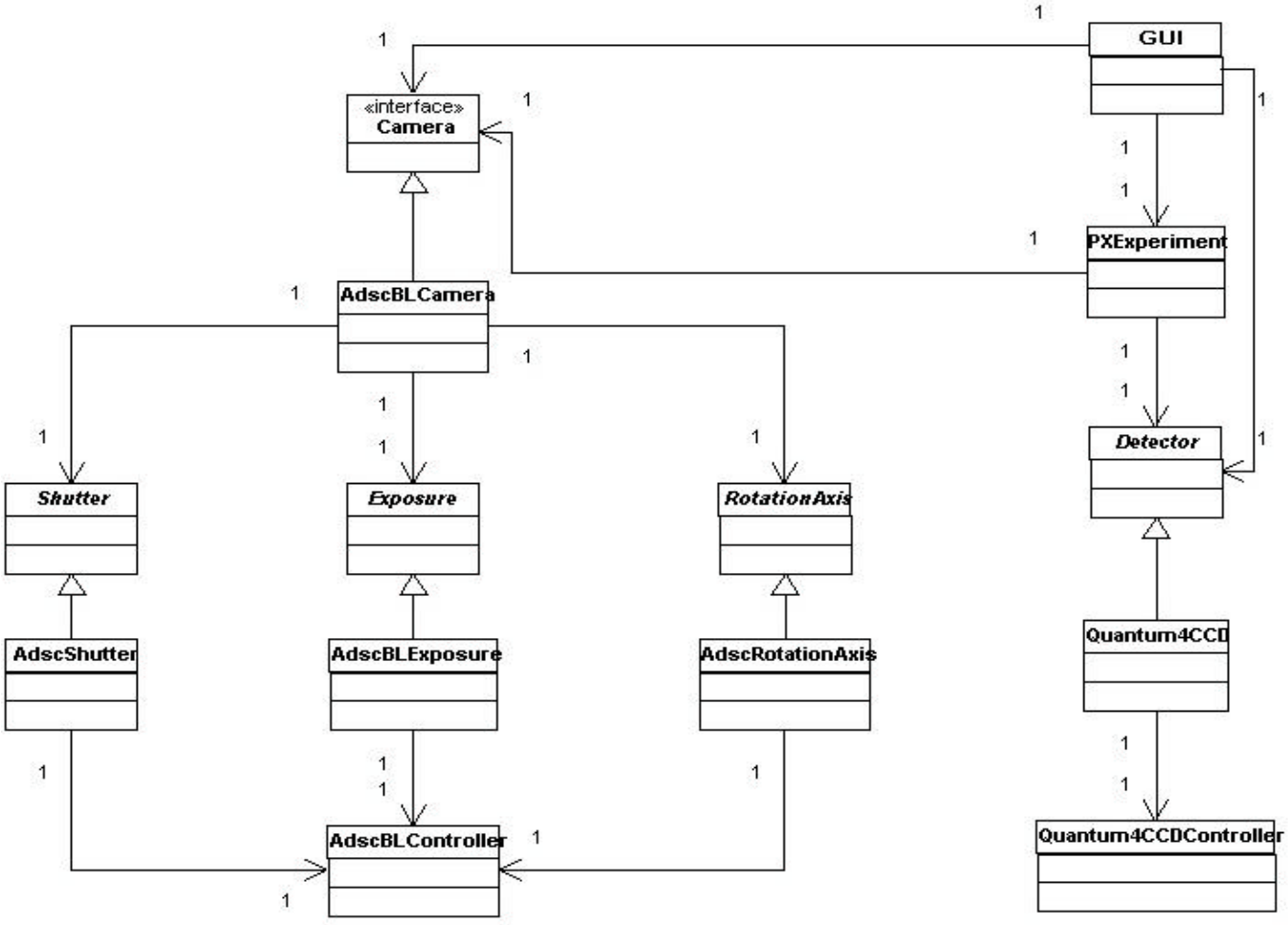
- Shared development effort allows more to be achieved without repetition.
- Other programmers understand the software.
- Wider use leads to greater robustness.
- Get benefits from aspects that may not at first be seen as directly PX aims e.g. scripting, XML configuration.
- Users see common interfaces across beam lines and stations.
- Aids the development of multiple technique stations.

PXGEN++

- Same GUI for data collection independent of detector in use.
- Data collection ready, tested with Q4 and MAR image plates (MAR CCD next).
- Using OEMove for beam line set-up.
- PXGEN++ and OEMove undergoing final tests.
- Once fully tested and released on one PX station should be able to deploy on others.
- Need to integrate in XAFS control, automation, sample changing etc.
- Standard XAFS GUI and control under development as part of 6.2 project (NCD, XRD and XAFS).


Exceed
Toolchest
Desktop
Selected
Internet
Find
System
Help
mardc
mardc: config: pixelsx set t
mardc: config: pixelsy set t
mardc: config: multiplier se
mardc: config: phisteps set
mardc: config: diststeps set
mardc: config: phitop set to
mardc: config: disttop set t
mardc: config: distmax set t
mardc: config: distmin set t
mardc: config: unitsec set t
mardc: config: unitdose set
mardc: config: wavelength se
mardc: config: usedistance s
mardc: config: usephi set to
mardc: config: flags set to
mardc: config: nc_pointer se
PXGEN++ (V1.1)
Quit
Setup
Beam Alignment
Beamline
Goniometer
Detector Distance
Detector Specific
Fluorescence Scan
Collect
Edit Exposures
Perform Exposures
Single Exposures
Abort Exposures
Expert System
Process
Processing GUI
Status
Shutter
Phi
0.0
Sample to Detector
100
Operation
ready
Progress to End
Feb 7, 2002 09:55
Detector Distance Setup
Required distance
0
mm
Present distance
100
Initialise
Set
Move
Dismiss
Single Axis Goniometer Se
Required angle
0
Present angle
0
Set
Move
+90 de
Edit Exposures
Data directory
/Local/shk/
Prefix filename
karen_
Detector Distance
100
mm
Wavelength
0.979
Angstrom
Number of Experiments
1
Start Phi
Phi Increment
Number of Images
Time
Template Number
10.0
1.0
1
5.0
0
Display every
0
th image.
Apply
Ok
Dismiss

Detectors and Cameras



Abstract Detector provides standard interface e.g.

•initialise()

•clear()

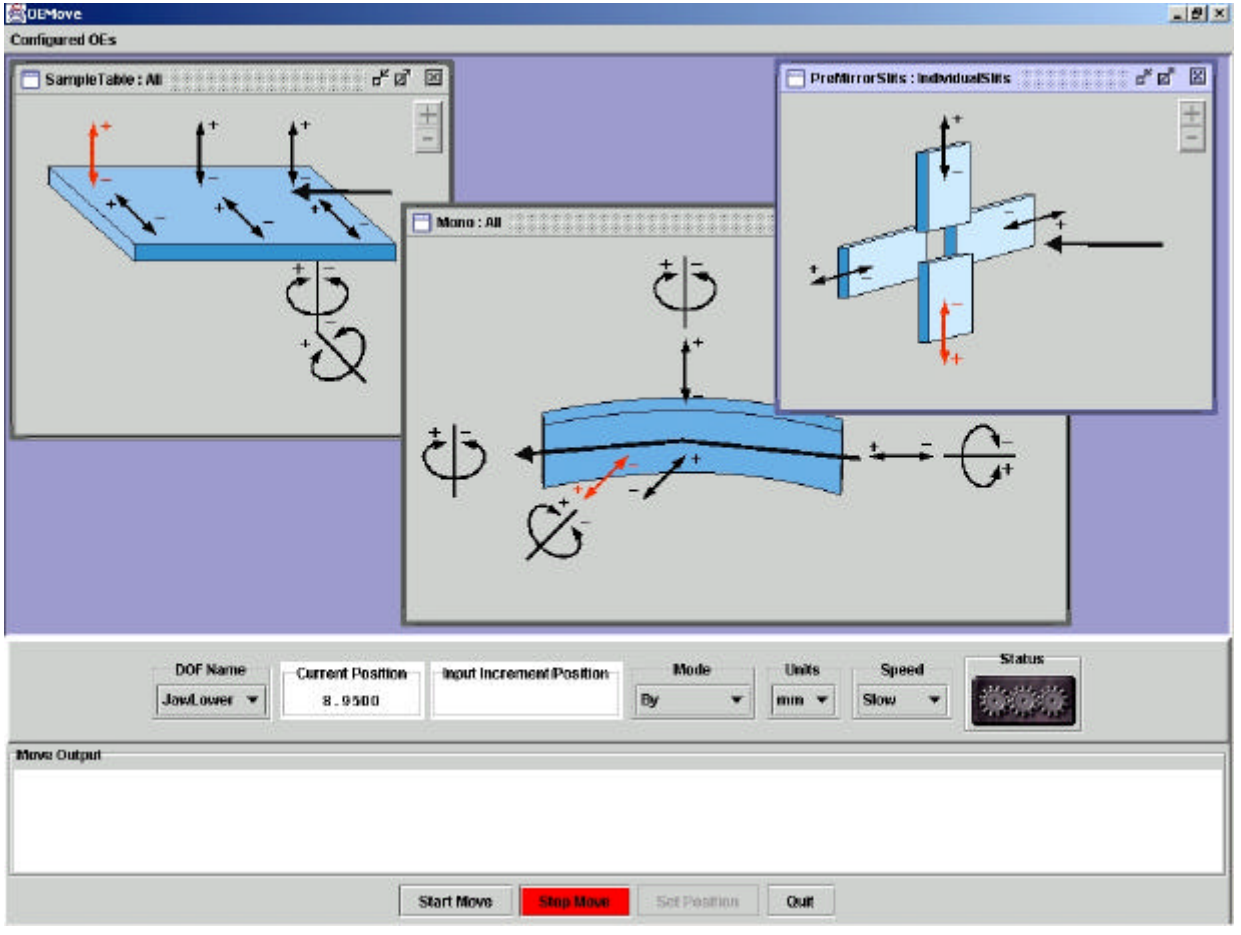
•read()…….

Concrete detectors implement these.

Similarly for Camera.

GUI/Experiment only know that they have a Detector and a Camera.

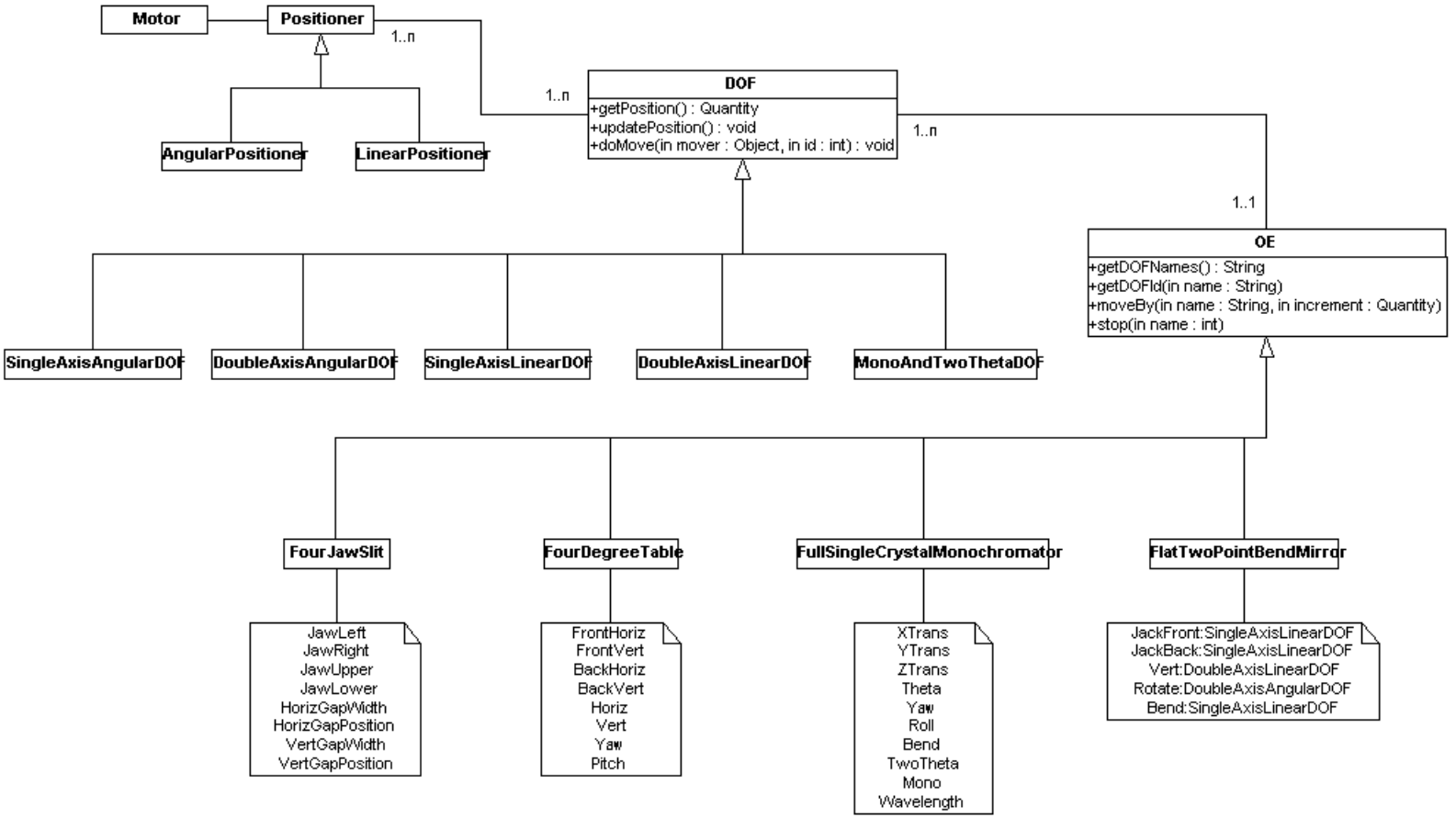
OEMove



- OEMove provides a standard tool to allow the control and set up of Optical Elements.
- OEedit allows the configuration of one or more visual representations of OEs.
- OEMove reads in representations at run time.
- One tool meets needs of PX and other stations.

Optical Elements

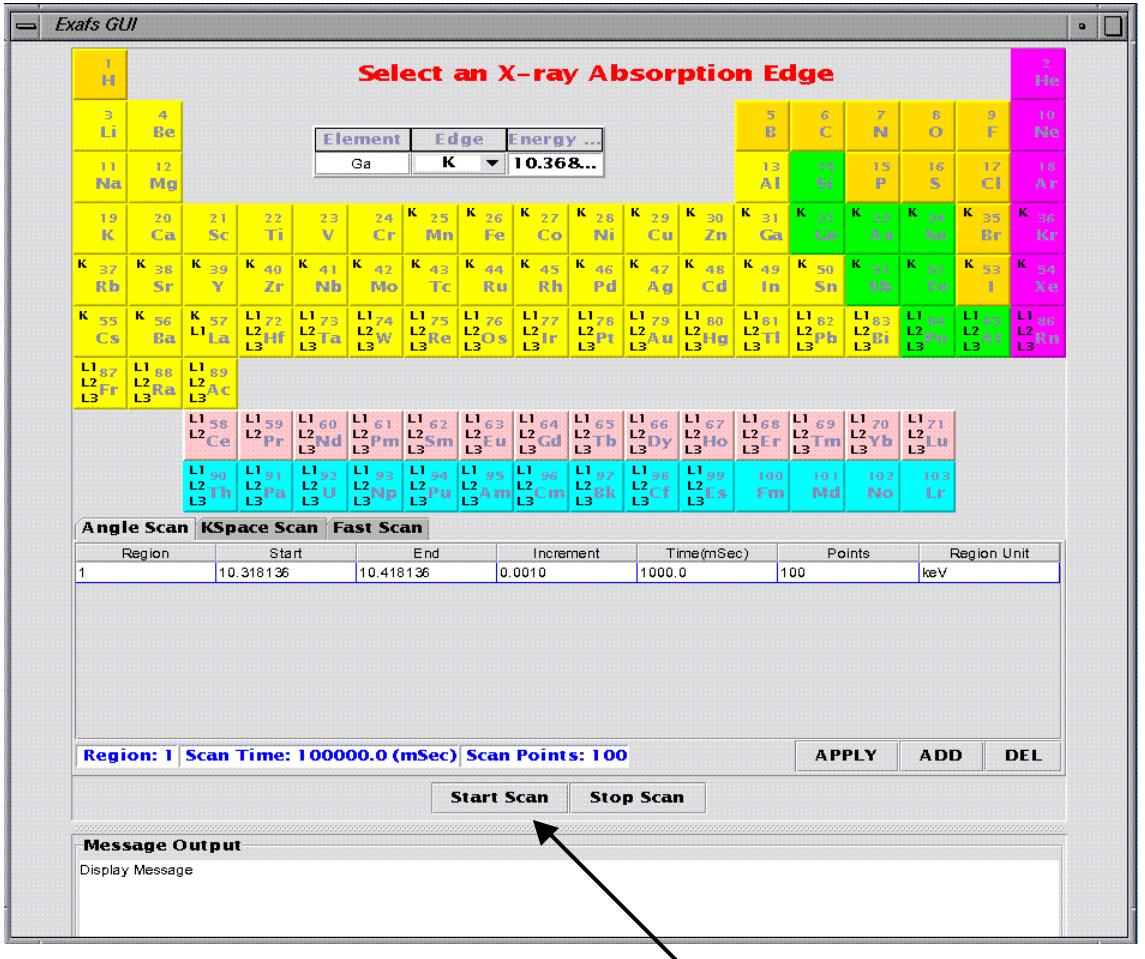
- OEs obey a standard interface.
- Each OE has a number of specific DOFs (Degree Of Freedom).
- Specific DOFs are implemented generally e.g. FrontHoriz and BackHoriz by SingleAxisLinearDOF.
- DOFs obey a standard interface.



Scripting - JCLAM

- JCLAM is a scripting language developed on top of JPython. A set of Python scripts basically.
- Can still use standard Python language.
- JCLAM run separately and accepts commands via a message handler.
- Separates control from the GUI.
- Standard scanning GUI will be set up.
- Allows easy/rapid alteration of control.
- Users can be given control of hardware and allowed to alter scans where required e.g. in different projects.
- Examples
    - pos LeftSlit 2.0 RightSlit 2.0
    - scan Slit 1 1 5 qcr 1

Absorption Edge Scans



- Standard absorption edge scan interface.
- Supports multiple modes, Angle, KSpace and Fast.
- GUI completely detached from control.
- Scans done via JCLAM.

scansie.SCANSIE(['mono',18235.3,-1.8,18054.2,'tm',1000.0])

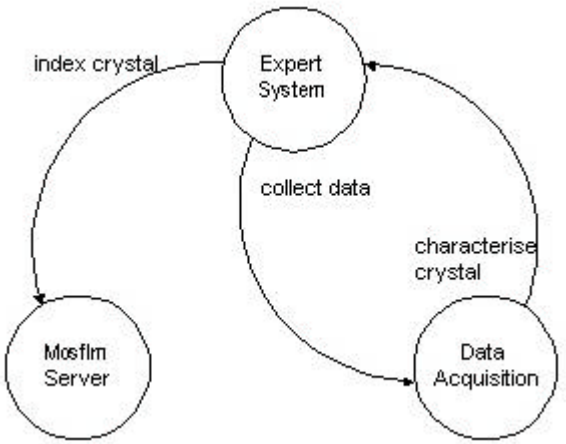
Automation

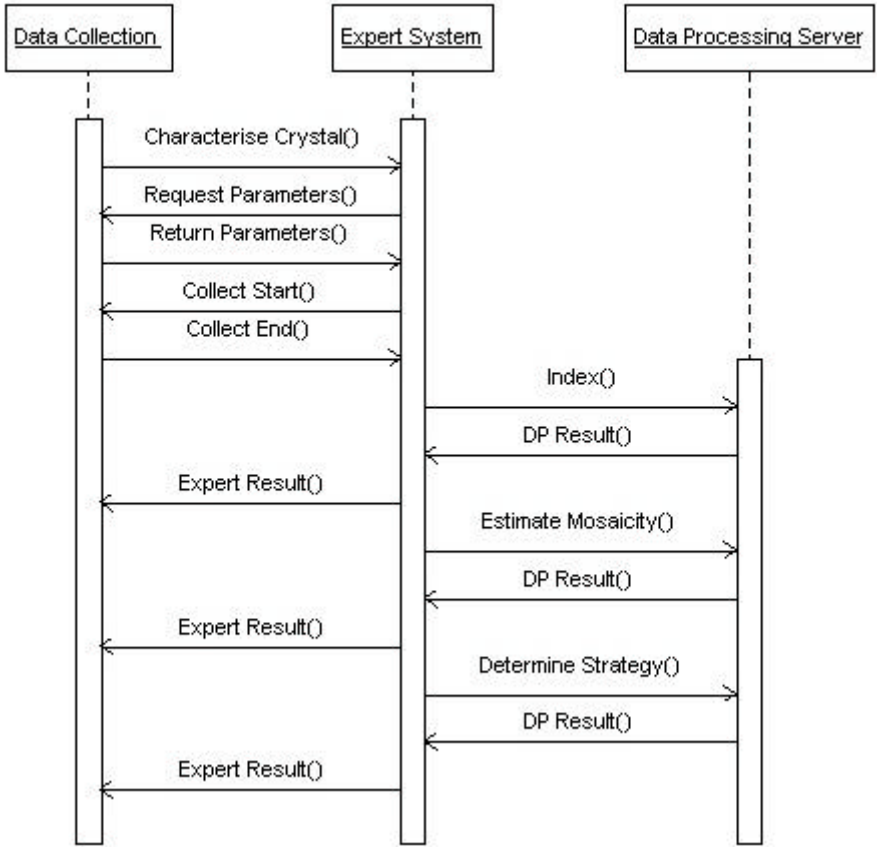
- Development of Optical Elements and the use of JCLAM should facilitate beam line automation.
  - Feedback required on beam
  - Objectives include
    - Alignment of camera to beam, standard peak searching and scanning.
    - Slit optimisation.
    - Focussing of mirror/monochromators.
    - Sample changing and alignment.
- Feedback from data processing (DNA).
- Automatic logging of data collection.

DNA - DNA’s Not Autostruct

- A collaboration presently involving Cambridge LMB, ESRF and Daresbury.
- Still at a relatively early stage and under active development (unfortunately part time).
- Eventual aim is to completely automate the collection and processing of Protein Crystallography data.
- Initially the project will develop what we are calling an 'expert system' sitting between data collection software at a given x-ray synchrotron and Mosflm.
- Utilising the Mosflm server under development at Cambridge for new Mosflm GUI.
- The project however also aims to allow the use of other data processing software in the long term.
- http://www.dna.ac.uk/

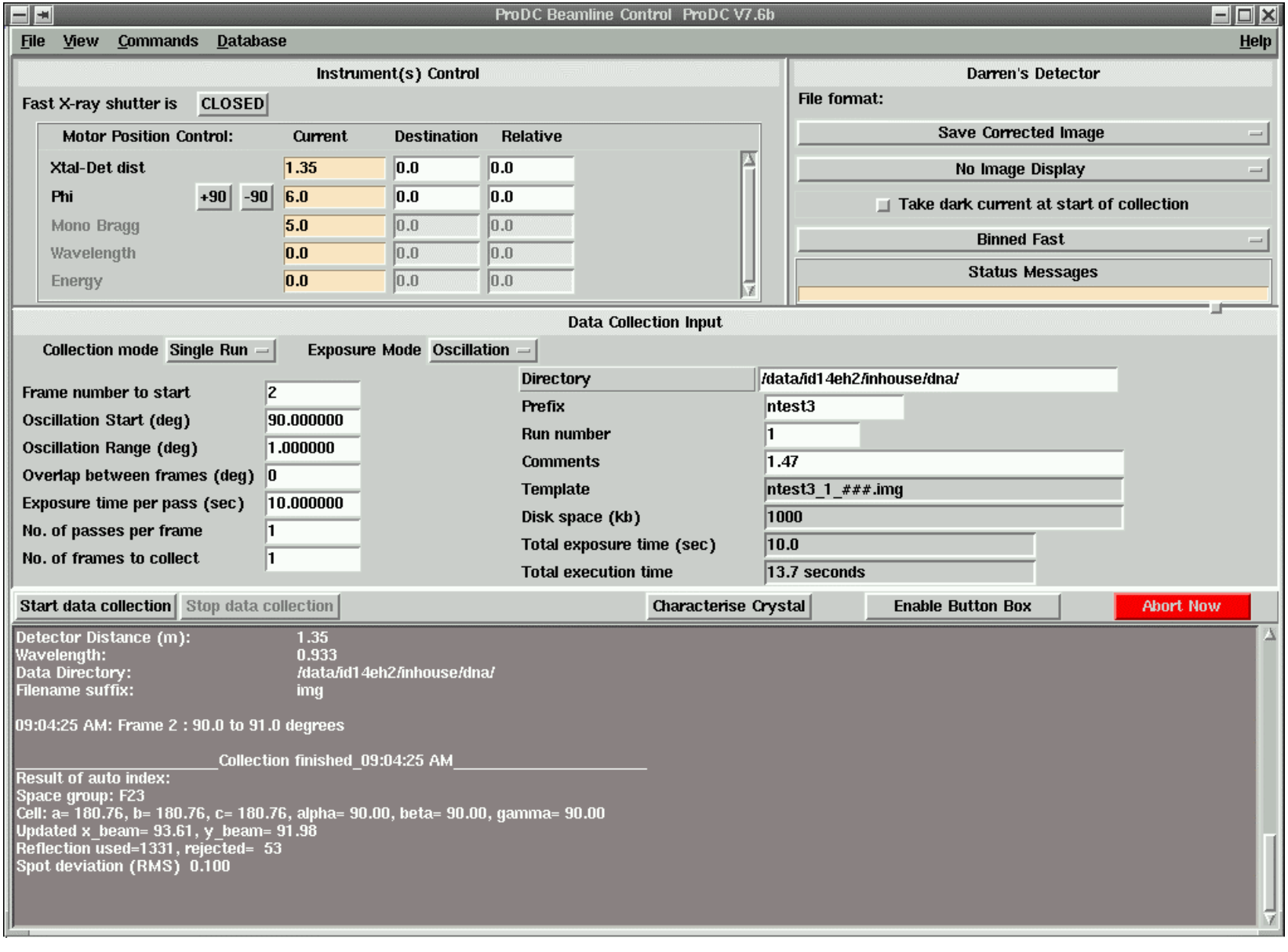
DNA architecture





DNA progress at ESRF

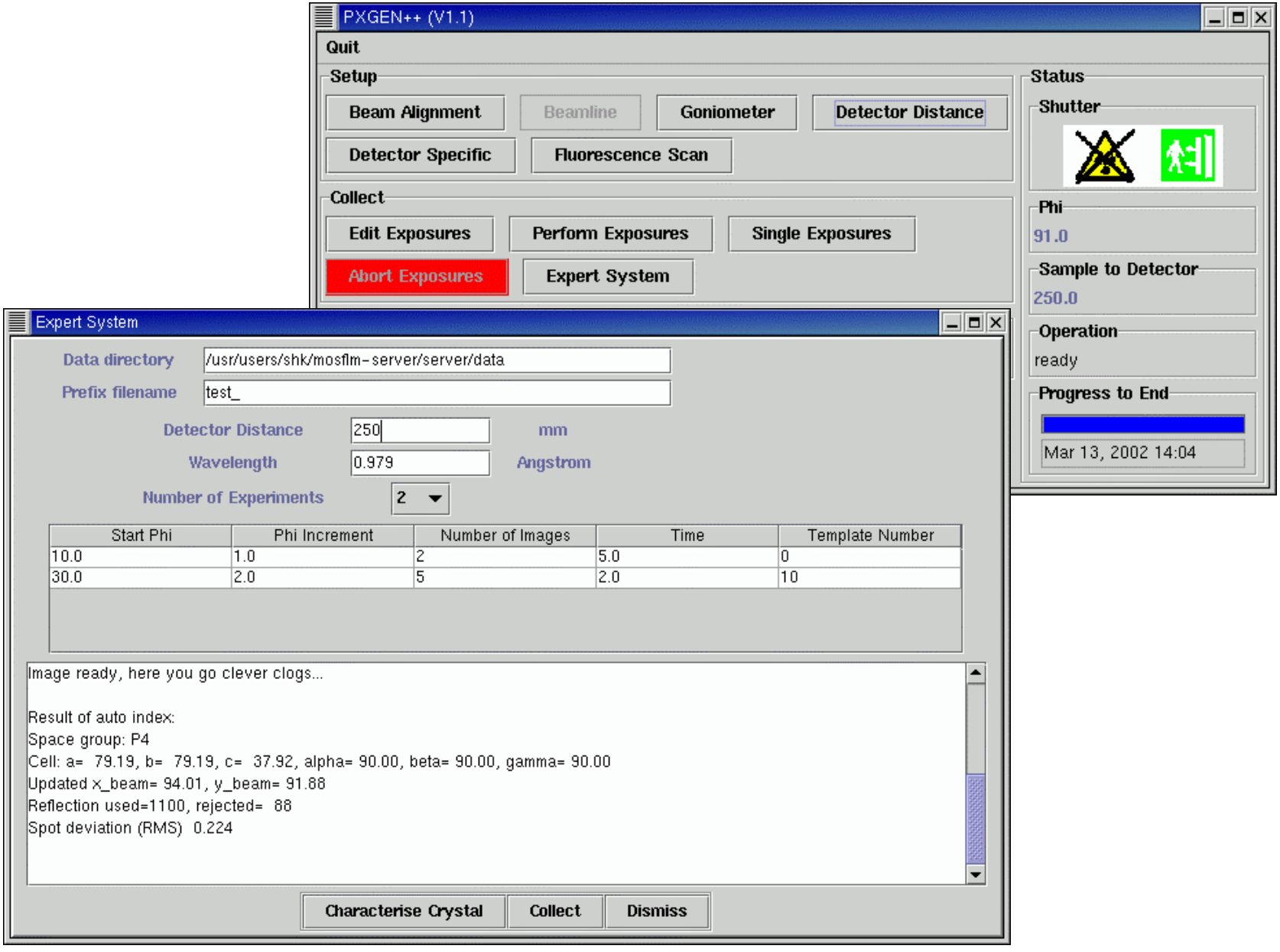
- ProDC modified to add a button, characterise crystal.
- Expert system developed to communicate with Mosflm server.
- ProDC communicates with Expert system.
- Communication to/from expert system and Mosflm server work.
- Crystal mounted on ID14.
- Characterisation collected two images on behalf of expert system.
- Expert system instigated auto-indexing of images by Mosflm via Mosflm server.
- Results relayed back to ProDC and displayed in message window.


ProDC Beamline Control ProDC V7.6b
File View Commands Database Help
Instrument(s) Control
Fast X-ray shutter is CLOSED
Motor Position Control: Current Destination Relative
Xtal-Det dist 1.35 0.0 0.0
Phi +90 -90 6.0 0.0 0.0
Mono Bragg 5.0 0.0 0.0
Wavelength 0.0 0.0 0.0
Energy 0.0 0.0 0.0
Darren's Detector
File format:
Save Corrected Image
No Image Display
Take dark current at start of collection
Binned Fast
Status Messages
Data Collection Input
Collection mode Single Run
Exposure Mode Oscillation
Frame number to start 2
Oscillation Start (deg) 90.000000
Oscillation Range (deg) 1.000000
Overlap between frames (deg) 0
Exposure time per pass (sec) 10.000000
No. of passes per frame 1
No. of frames to collect 1
Directory /data/id14eh2/inhouse/dna/
Prefix ntest3
Run number 1
Comments 1.47
Template ntest3_1_###.img
Disk space (kb) 1000
Total exposure time (sec) 10.0
Total execution time 13.7 seconds
Start data collection
Stop data collection
Characterise Crystal
Enable Button Box
Abort Now
Detector Distance (m): 1.35
Wavelength: 0.933
Data Directory: /data/id14eh2/inhouse/dna/
Filename suffix: img
09:04:25 AM: Frame 2 : 90.0 to 91.0 degrees
Collection finished_09:04:25 AM
Result of auto index:
Space group: F23
Cell: a= 180.76, b= 180.76, c= 180.76, alpha= 90.00, beta= 90.00, gamma= 90.00
Updated x_beam= 93.61, y_beam= 91.98
Reflection used=1331, rejected= 53
Spot deviation (RMS) 0.100

DNA progress at DL

- Stand alone GUI Built
- Can use GUI from PXGEN++
  - Will contain results of strategy calculation and allow modification before data collection
- Expert system used as developed at ESRF
- Java class written to interface to expert system
- Communication to/from same expert system works
- XML parsing via castor, http://castor.exolab.org

```
Object o = unmarshaller.unmarshal(new StringReader(command));
CollectStart cs = (CollectStart) o;
```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Detector Specific
Fluorescence Scan
Collect
Edit Exposures
Perform Exposures
Single Exposures
Abort Exposures
Expert System
Status
Shutter
Phi
91.0
Sample to Detector
250.0
Operation
ready
Progress to End
Mar 13, 2002 14:04
Expert System
Data directory
/usr/users/shk/mosflm-server/server/data
Prefix filename
test_
Detector Distance
250
mm
Wavelength
0.979
Angstrom
Number of Experiments
2
Start Phi
Phi Increment
Number of Images
Time
Template Number
10.0
1.0
2
5.0
0
30.0
2.0
5
2.0
10
Image ready, here you go clever clogs...
Result of auto index:
Space group: P4
Cell: a= 79.19, b= 79.19, c= 37.92, alpha= 90.00, beta= 90.00, gamma= 90.00
Updated x_beam= 94.01, y_beam= 91.88
Reflection used=1100, rejected= 88
Spot deviation (RMS) 0.224
Characterise Crystal
Collect
Dismiss

Acknowledgements

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ESRF

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Cambridge

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